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COMPUTED STRUCTURE OF GRAIN BOUNDARIES COMPARED WITH TEM OBSERVATIONS

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Employing computer simulation techniques several studies of the relaxation of atoms in coincidence type grain boundaries have been performed in recent years. Often it is difficult to obtain a clear representation of the relaxed boundary structure, especially in the case of small atomic displacements. In this paper a method of representing the relaxed grain boundary structure is described using a Fourier analysis of the atomic configuration after relaxation. Computer experiments were carried out on $\Sigma = 19$, 46.8°/[111] in Al. Next, results obtained from computer experiments dealing with the interaction between He and a tilt grain boundary in Mo are presented. Direct motivation for this study stems from the transmission electron microscopic observation of helium trapping at a set of [100] edge dislocations defining a low angle tilt boundary in Mo.

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EFFECT OF SECONDARY RELAXATIONS ON DIFFRACTION FROM HIGH-Σ [001] TWIST BOUNDARIES

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The types of diffraction effects which may be expected from secondary relaxations in high-Σ [001] twist boundaries are calculated and discussed. An idealized two-plane model is used which incorporates secondary relaxations by rotating patches of boundary about coincident site lattice elements normal to the boundary. Local relaxations within the patches are also employed using rotational relaxations about local O-lattice elements in a manner consistent with earlier results. The main effect of secondary relaxations is the splitting of grain boundary reflections into small clusters which fall on a "grain boundary dislocation lattice". This localized splitting is significant only when the deviation of the boundary from a nearby low-Σ misorientation becomes sufficiently large. Under these circumstances a noticeable distortion of the diffraction pattern can also occur. The results are compared with some X-ray diffraction observations from twist boundaries in gold.